

Absence of Singularity in Loop Quantum Cosmology

Martin Bojowald*

*Center for Gravitational Physics and Geometry, The Pennsylvania State University,
104 Davey Lab, University Park, PA 16802, USA*

It is shown that the cosmological singularity in isotropic minisuperspaces is naturally removed by quantum geometry. Already at the kinematical level, this is indicated by the fact that the inverse scale factor is represented by a bounded operator even though the classical quantity diverges at the initial singularity. The full demonstration comes from an analysis of quantum dynamics. Because of quantum geometry, the quantum evolution occurs in *discrete* time steps and does not break down when the volume becomes zero. Instead, space-time can be extended to a branch preceding the classical singularity independently of the matter coupled to the model. For large volume the correct semiclassical behavior is obtained.

On a macroscopic scale, the gravitational field is successfully described by general relativity, which is experimentally well tested in the weak field regime. However, this classical theory must break down in certain situations where it predicts singularities, i.e. boundaries of space-time which can be reached by observers in finite proper time, but beyond which an extension of the space-time manifold is impossible [1]. An outstanding example is the big-bang singularity appearing in cosmological models. At this point curvature diverges whence the classical theory completely breaks down and has to be replaced by a quantum theory of gravity. However, up to now there is no complete quantum theory of gravity, and so the problem has been approached by first carrying out a symmetry reduction (by requiring isotropy and homogeneity) and then quantizing the resulting minisuperspace models which have only a finite number of degrees of freedom [2,3]. In the context of these models, as yet, there is no definitive resolution of the status of the initial singularity. Furthermore, generally the methods used in this analysis can easily miss some key features of the full theory. Indeed, while it has been speculated for a long time that quantum gravity may lead to a *discrete structure* of space and time which could cure classical singularities, it has not been possible to embody this idea in standard quantum cosmological models.

By now, there are promising candidates for a quantum theory of gravity. The results reported in this letter are obtained in the framework of quantum geometry [4] which *does* predict a discrete geometry because, e.g., the spectra of geometric operators as area and volume are discrete [5–7]. Although temporal observables have not been included in the *full* theory, it is clear that the space-time structure is very different from that used in general relativity. But this difference can be important only at very short scales or in high curvature regimes like the one close to the classical singularity. This leads to the basic question raised here: *What happens to the classical cosmological singularity in quantum geometry?*

The first step in our approach is the construction of

isotropic states in full quantum geometry; we *first* quantize and *then* carry out a symmetry reduction. This, however, is not a straightforward problem because the discrete structure of space, represented by a graph (spin network) embedded in space, necessarily breaks any continuous symmetry. But symmetric states can be defined as generalized states of quantum geometry [8] which can be used for a reduction to minisuperspace models [9]. Note that this is not a standard symmetry reduction of the classical theory because symmetric states are interpreted as generalized states in the *full* kinematical quantum theory. Only the Hamiltonian constraint has to be quantized and solved after the reduction. An immediate and striking consequence is that, in contrast to standard quantum cosmological models, spatial Riemannian geometry is discrete leading to a discrete volume spectrum [10]. Furthermore, in contrast to standard quantum cosmology, the same techniques as in the full theory [11] can be used for the quantization of the reduced Hamiltonian constraint of the cosmological models [12]. This implies another difference, namely that the evolution equation is not a differential equation in time, but a *difference equation* manifesting the discreteness of time [13].

Structure of isotropic models. According to [8,9] states for isotropic models in the connection representation are distributional states of the full kinematical quantum theory supported on isotropic connections of the form $A_a^i = c\Lambda_I^i \omega_a^I$ where Λ_I is an internal $SU(2)$ -dreibein and ω^I are the left-invariant one-forms on the “translational” part of the symmetry group acting on the space manifold Σ . The momenta are densitized triads of the form $E_i^a = p\Lambda_I^i X_I^a$ with left-invariant densitized vector fields X_I fulfilling $\omega^I(X_J) = \delta_J^I$. Besides gauge freedom, there are only the two canonically conjugate variables $\{c, p\} = \kappa\gamma/3$ ($\kappa = 8\pi G$ is the gravitational constant and $\gamma > 0$ the Barbero–Immirzi parameter) which have the physical meaning of extrinsic curvature and square of radius ($a = \sqrt{|p|}$ is the scale factor). The kinematical Hilbert space $\mathcal{H}_{\text{kin}} = L^2(SU(2), d\mu_H)$ is the space of functions of isotropic connections which are square inte-

grable with respect to Haar measure. Orthonormal gauge invariant states are (see [10] for details)

$$\chi_j = \frac{\sin(j + \frac{1}{2})c}{\sin \frac{c}{2}}, \quad \zeta_j = \frac{\cos(j + \frac{1}{2})c}{\sin \frac{c}{2}} \quad (1)$$

for $j \in \frac{1}{2}\mathbb{N}_0$ together with $\zeta_{-\frac{1}{2}} = (\sqrt{2} \sin \frac{c}{2})^{-1}$. These states are eigenstates of the volume operator \hat{V} with eigenvalues [10]

$$V_j = (\gamma l_P^2)^{\frac{3}{2}} \sqrt{\frac{1}{27} j(j + \frac{1}{2})(j + 1)}. \quad (2)$$

Later we will also use a different orthonormal basis of states adapted to the triad by introducing

$$|n\rangle := \frac{\exp(in\frac{c}{2})}{\sqrt{2} \sin \frac{c}{2}}, \quad n \in \mathbb{Z} \quad (3)$$

where n represents the eigenvalues of p which determines the dreibein. In contrast to j , which is always positive and represents eigenvalues of the square of the scale factor, n can also be negative. For this it is important that we have not only the character functions χ_j , but also the additional functions ζ_j . This concludes the discussion of quantum states.

The inverse scale factor. Classically, the metric of an isotropic spatial slice is given by $q_{IJ} = a^2 \delta_{IJ} = e_I^i e_J^i$ where e_I^i is the co-triad. From this quantity we can build the expression

$$m_{IJ} := \frac{q_{IJ}}{\sqrt{\det q}} = \frac{e_I^i e_J^i}{|\det e|} = \frac{1}{a} \delta_{IJ}$$

for the inverse scale factor, which we now quantize as a first application of the previously derived calculus. The co-triad is not a fundamental variable, but it can be quantized to $2i(\gamma l_P^2)^{-1} h_I [h_I^{-1}, \hat{V}]$ due to the classical identity $e_a^i = 2(\kappa\gamma)^{-1} \{A_a^i, V\}$ [11]. The expression $\det e$ in the denominator of m_{IJ} can be quantized to the volume operator which then can be absorbed into the commutators. Such a procedure has already been applied in [14] in order to quantize matter Hamiltonians which become densely defined operators, and in the same way we arrive at the *bounded* operator

$$\begin{aligned} m_{IJ} &= \frac{32}{\gamma^2 l_P^4} \text{tr} \left(h_I \left[h_I^{-1}, \sqrt{\hat{V}} \right] h_J \left[h_J^{-1}, \sqrt{\hat{V}} \right] \right) \\ &= \frac{64}{\gamma^2 l_P^4} \left(\left(\sqrt{\hat{V}} - \cos \frac{c}{2} \sqrt{\hat{V}} \cos \frac{c}{2} - \sin \frac{c}{2} \sqrt{\hat{V}} \sin \frac{c}{2} \right)^2 \right. \\ &\quad \left. - \delta_{IJ} \left(\sin \frac{c}{2} \sqrt{\hat{V}} \cos \frac{c}{2} - \cos \frac{c}{2} \sqrt{\hat{V}} \sin \frac{c}{2} \right)^2 \right). \end{aligned}$$

This operator is simultaneously diagonalizable with the volume operator and has the eigenvalues

$$\begin{aligned} m_{IJ,j} &= \frac{16}{\gamma^2 l_P^4} \left(4 \left(\sqrt{V_j} - \frac{1}{2} \sqrt{V_{j+\frac{1}{2}}} - \frac{1}{2} \sqrt{V_{j-\frac{1}{2}}} \right)^2 \right. \\ &\quad \left. + \delta_{IJ} \left(\sqrt{V_{j+\frac{1}{2}}} - \sqrt{V_{j-\frac{1}{2}}} \right)^2 \right) \end{aligned} \quad (4)$$

$$\sim V^{-\frac{1}{3}} \left(\delta_{IJ} + \frac{\gamma^2}{9} \left(\frac{1}{256} + \frac{37}{192} \delta_{IJ} \right) \frac{l_P^4}{a^4} \right) \quad (5)$$

where in the second step we have assumed that j — and hence V_j — is large. Thus, for large j , the leading term is the classical value $V^{-\frac{1}{3}} \delta_{IJ}$, and the corrections (which are not necessarily isotropic) are of only the fourth order. We see that our quantization leading to a bounded operator does not spoil the classical limit. In fact, the a^{-1} -behavior can be observed in a range which is much larger than expected from the large- j expansion. As Fig. 1 demonstrates, even for $j = 1$ are the eigenvalues very close to the classical expectation, and only the lowest three eigenvalues show large deviations. But this is already deeply in the quantum regime, so such deviations are expected and lead to a finite behavior of the classically diverging m_{II} . Note that the volume operator has the eigenvalue zero (three-fold degenerate), but even in the corresponding eigenstates is the quantization of the inverse scale factor perfectly finite. This may be taken as a first indication for a removal of the classical singularity, although only at the kinematical level.

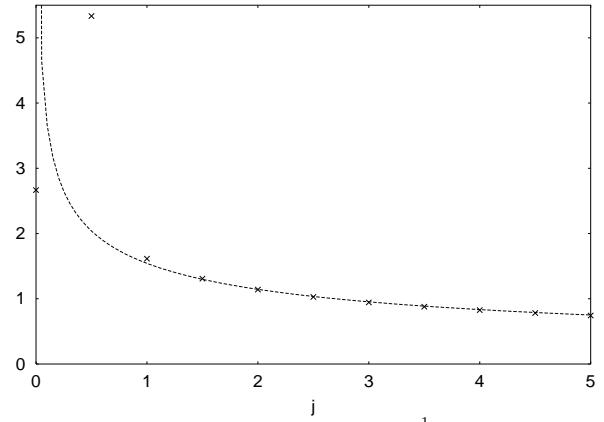


FIG. 1. The classical expectation $V_j^{-\frac{1}{3}}$ (dashed line) and eigenvalues $m_{II,j}$, $j \geq 0$ of the inverse scale factor (\times). Contrary to the classical curve, the latter peak at $j = \frac{1}{2}$ and decrease for $j = 0$ and $j = -\frac{1}{2}$ ($m_{II,-\frac{1}{2}} = 0$ is not shown).

Discrete time evolution. Following the basic steps of the quantization in the full theory [11], the Hamiltonian constraints for cosmological models can be quantized with some adaptations to the symmetry [12]. For simplicity we write down here only the key term, the so-called Euclidean term $H^{(E)}$, of the constraint operator for spatially flat isotropic models. However, all our qualitative results remain true for the full constraint and also for isotropic models with positive curvature. The constraint is of the form

$$\begin{aligned} \hat{H}^{(E)} &= \frac{4i}{\gamma \kappa l_P^2} \sum_{IJK} \epsilon^{IJK} \text{tr} (h_I h_J h_I^{-1} h_J^{-1} h_K [h_K^{-1}, \hat{V}]) \\ &= -\frac{96i}{\gamma \kappa l_P^2} \sin^2 \frac{c}{2} \cos^2 \frac{c}{2} (\sin \frac{c}{2} \hat{V} \cos \frac{c}{2} - \cos \frac{c}{2} \hat{V} \sin \frac{c}{2}) \end{aligned}$$

with action

$$\hat{H}^{(E)}|n\rangle = -\frac{3}{\gamma\kappa l_P^2}(V_{|n|/2} - V_{|n|/2-1}) \times (|n+4\rangle - 2|n\rangle + |n-4\rangle). \quad (6)$$

In order to “unfreeze dynamics” and interpret solutions as “evolving states,” as usual [15,16] we have to introduce an internal time which we choose as the dreibein coefficient p . Accordingly, we transform states $|s\rangle$ into an adapted representation by expanding $|s\rangle = \sum_n s_n |n\rangle$ in eigenstates $|n\rangle$ of p . This will allow us to find an interpretation of physical states as evolving histories. Furthermore, discrete geometry implies that eigenvalues of p are discrete, whence time evolution is now discrete (see [13] for details). Moreover, since we chose a geometrical quantity as time which can be negative and is zero for vanishing volume, we will be able to test the possibility of a quantum evolution through the classical singularity.

To realize dynamics, we need to extend the model with matter degrees of freedom which can evolve with this internal time. Matter can be incorporated by using coefficients $s_n(\phi)$ depending on the matter field ϕ in an appropriate fashion, the details of which is not important for what follows. The Hamiltonian constraint can then be written down using a matter Hamiltonian \hat{H}_ϕ (as in [14]) which is diagonal in the gravitational degrees of freedom (and can also contain a cosmological term). The resulting quantum constraint equation can then be regarded as an evolution in discrete time:

$$(V_{|n+4|/2} - V_{|n+4|/2-1})s_{n+4}(\phi) - 2(V_{|n|/2} - V_{|n|/2-1})s_n(\phi) + (V_{|n-4|/2} - V_{|n-4|/2-1})s_{n-4}(\phi) = \frac{1}{3}\gamma\kappa l_P^2 \hat{H}_\phi s_n(\phi) \quad (7)$$

(V_j are the eigenvalues (2) of the volume operator with $V_{-1} = 0$) which is a difference equation for the coefficients $s_n(\phi)$ depending on the discrete label n (our discrete time).

Fate of the singularity. Given initial data $s_n(\phi)$ for some negative n , we can use (7) in order to determine later values for higher n . This, however, is possible only as long as the highest order coefficient $V_{|n+4|/2} - V_{|n+4|/2-1}$ is nonzero, which is the case if and only if $n \neq -4$. So all coefficients for $n < -4$ are determined by the initial data. However, (7) does not determine s_0 and instead leads to a *consistency condition* for the initial data. So the quantum evolution appears to break-down just at the classical singularity, i.e. at the zero eigenvalue of p . But this is not the case; in fact all s_n for $n > 0$ are determined by (7) from the initial data. This occurs because for $n = 0$ we have: i) $V_{|n|/2} - V_{|n|/2-1} = 0$, and ii) $\hat{H}_\phi s_n(\phi) = 0$; thus s_0 completely drops out of the iterative evolution. E.g., s_4 is determined solely by s_{-4} because the coefficient of s_n vanishes for $n = 0$. So we can evolve through the singularity and determine all s_n for $n \neq 0$. (The vanishing of $\hat{H}_\phi s_0(\phi)$ follows from

the quantization of matter Hamiltonians [14] similarly as described for the inverse scale factor.)

Of course, in order to determine the complete state we also have to know s_0 , but a closer analysis reveals that s_0 is fixed from the outset: The Hamiltonian constraint always has the eigenstate $s_n = s_0 \delta_{n0}$ with zero eigenvalue which is completely degenerate and not of physical interest. All evolving solutions are orthogonal to this state and have $s_0 = 0$ which already fixes the coefficient s_0 left undetermined by using the evolution equation. We see that the complete state is determined by initial data for negative n , and so there is no singularity in isotropic loop quantum cosmology. The intuitive picture is as follows: Since for $n < 0$ the volume eigenvalues $V_{(|n|-1)/2}$ decrease with increasing n , there is a contracting branch for negative n leading to a state of zero volume (in general, $s_{\pm 1} \neq 0$ and the volume vanishes for $n = \pm 1$ which corresponds to $j = 0$) in which the universe bounces off leading to the expanding branch for positive n which only can be seen in the classical theory and in standard quantum cosmology. This conclusion holds true for any kind of matter and cosmological constant, and is a purely quantum gravitational effect. In particular, we do not need to introduce matter violating energy conditions and thereby evade the singularity theorems. However, our result crucially depends on the factor ordering of the constraint which was chosen as one of the *standard* possibilities ordering all triad components to the right.

The semiclassical regime. We have seen that the classical singularity is removed in loop quantum cosmology. But we need more for a viable cosmological model, namely we also need the correct behavior in the semiclassical regime. Classical behavior can only be present for large volume and small extrinsic curvature, i.e. if $|n|$ is large, c is small and the wave function does not vary strongly between successive times n (otherwise the state would have access to the Planck scale). In this regime we can interpolate between the discrete labels n and define a wave function $\psi(a) := s_{n(a)}$, $n(a) := 6a^2/\gamma l_P^2$ with a ranging over a continuous range (using $a = \sqrt{|p|} \sim \sqrt{\gamma l_P} \sqrt{|n|/6}$ for large $|n|$ as interpolation points). The difference operator Δ then becomes $(\Delta s)_n := s_{n+1} - s_{n-1} = \frac{1}{6}\gamma l_P^2 a^{-1} d\psi/da + O(l_P^5/a^5)$ leading to an approximate constraint operator $\hat{H}^{(E)} \sim -96(i\Delta/2)^2 \cdot a/4 \sim -6\gamma^2 l_P^4 (-\frac{i}{3}d/d(a^2))^2 a$ for large a . This is exactly what one obtains from the classical constraint $H^{(E)} = -6c^2 \sqrt{|p|}$ in standard quantum cosmology [17] by quantizing $3\hat{c} = -i\gamma l_P^2 d/dp$. In our framework, however, this is only an approximate equation valid for large scale factors. For this equation one can use WKB-techniques in order to derive the correct classical behavior.

Going to smaller a one has to include more and more corrections in the expansion of the difference operators and also of the volume eigenvalues. By doing so one can

derive perturbative corrections for an effective Hamiltonian including higher derivative terms. The closer we come to the classical singularity, the more corrections we have to include; and at the singularity we need to know all corrections which, as we know from our non-perturbative solution, have to add up to yield the discrete time behavior. So in these models higher order terms arise from the non-locality in discrete time of the fundamental theory. But even knowing all perturbative corrections, it would be very hard to see the correct behavior without knowing the non-perturbative quantization.

Quantum Euclidean space. In the simplest case, the Euclidean constraint for a spatially flat model without matter, it is possible to find an explicit solution to the constraint. The constraint equation is of order eight with one consistency condition as described above, so one expects seven independent solutions. But we are interested only in solutions which have a classical regime in the previous sense, i.e. no strong dependence on j for large j . Under this condition one can see that there is a unique (up to a constant factor) solution

$$\psi(c) = \sum_j \frac{2j+1}{V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}}} \chi_j(c) \quad (8)$$

in the connection representation. In standard quantum cosmology the constraint equation is $\hat{c}^2 \sqrt{|\hat{p}|} \xi(c) = 0$ with a solution $\sqrt{|\hat{p}|} \xi(c) = \delta(c)$ which is not unique. In order to compare the solutions we quantize a by $\hat{a} \chi_j = 2i(\gamma_P^2)^{-1}(V_{j+\frac{1}{2}} - V_{j-\frac{1}{2}})\chi_j$ leading to $\hat{a}\psi \propto \sum_j (2j+1)\chi_j$ which in fact is the delta function on the configuration space $SU(2)$. Therefore, we have a unique solution which incorporates the characterization of Euclidean space to have vanishing extrinsic curvature of its flat spatial slices.

Conclusions. We have shown in this paper that canonical quantum gravity is well-suited to analyze the behavior close to the classical singularity. For this, it is important to use only techniques which are applicable in the *full* theory. This leads to a discrete structure of space and time which cannot be seen in standard quantum cosmology. In our framework, the standard quantum cosmological description arises only as a limit for large volume where the discreteness is unimportant. For small volume, quantum geometry leads to new effects which are responsible for the removal of the classical singularity. In contrast to earlier attempts this is *not* achieved by introducing matter which violates energy conditions; it is a pure quantum gravity effect. It also does not avoid the zero volume state present in the classical singularity because in general the wave function is not orthogonal to states with zero volume eigenvalue. Nevertheless there is no sign of a singularity because in quantum geometry it is possible to have vanishing volume but non-diverging inverse scale factor, which in isotropic models dictates

all curvature blow-ups. Besides removing the singularity, the fact that an evolution through a state of zero volume is possible without problems could lead to topology change in quantum gravity. Technically, the removal of the singularity is achieved by using Thiemann's strategy [11] of absorbing inverse powers of \hat{V} into a Poisson bracket which also lead to densely defined matter Hamiltonians [14]. So it is the same mechanism which regularizes ultraviolet divergences in matter field theories and which removes the classical cosmological singularity. We have also seen that non-perturbative effects are solely responsible for this behavior and a purely perturbative analysis could not lead to these conclusions.

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* E-mail address: bojowald@gravity.phys.psu.edu

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